

A cold spectroscopic study on metal ion–benzo-crown ether complexes in the gas phase

Yoshiya Inokuchi

*Department of Chemistry, Graduate School of Sciences, Hiroshima University,
Kagamiyama 1-3-1, Higashi-Hiroshima, Hiroshima 739-8526, Japan
y-inokuchi@hiroshima-u.ac.jp*

In biological systems cyclic peptides such as gramicidin play important roles in carrying metal ions through biological membranes with high selectivity. Our target molecules in this study are crown ethers, which are much simpler hosts than biological ionophores but also have ion selectivity in solution. Despite their importance as host molecules having the ion selectivity, the origin of their functionality has not been fully understood at the molecular level; our final goal is to reveal the origin of the guest selectivity by spectroscopic methods. In this study we produce cold metal ion–benzo-crown ether complexes in vacuum by using an electrospray ion source and a cold ion trap, and perform UV photodissociation and IR-UV double-resonance spectroscopy. The cooling of the complexes up to ~10 K results in very sharp vibronic bands in their UV spectra, which enables us to measure conformer-specific IR spectra by using IR-UV experiments and to determine their structures. We will discuss the relation between the ion selectivity in solution and the structure and the number of the conformers on the basis of the spectroscopic results.

References

- [1] Y. Inokuchi et al., "UV and IR Spectroscopic Studies of Cold Alkali Metal Ion-Crown Ether Complexes in the Gas Phase", *J. Am. Chem. Soc.* **2011**, *133*, 12256-12263.
- [2] Y. Inokuchi et al., "Ion Selectivity of Crown Ethers Investigated by UV and IR Spectroscopy in a Cold Ion Trap", *J. Phys. Chem. A* **2012**, *116*, 4057-4068.
- [3] Y. Inokuchi et al., "Laser Spectroscopic Study of Cold Host-Guest Complexes of Crown Ethers in the Gas Phase", *ChemPhysChem* **2013**, *14*, 649-660.
- [4] Y. Inokuchi et al., "Microhydration Effects on the Encapsulation of Potassium Ion by Dibenzo-18-Crown-6", *J. Am. Chem. Soc.* **2014**, *136*, 1815-1824.